

09/885950

=> d his

(FILE 'HOME' ENTERED AT 14:43:22 ON 22 DEC 2001)

FILE 'CAPLUS' ENTERED AT 14:43:32 ON 22 DEC 2001
E WO 0190106/PN
E WO 200190106/PN

L1 1 S E3
SELECT L1 1 RN

FILE 'REGISTRY' ENTERED AT 14:44:54 ON 22 DEC 2001
L2 31 S E1-31
L3 1 S L2 AND C16H21F2NO2/MF

FILE 'CAOLD' ENTERED AT 14:48:20 ON 22 DEC 2001
L4 0 S L3

FILE 'BEILSTEIN' ENTERED AT 14:48:33 ON 22 DEC 2001
L5 0 S L3
L6 0 S L3 SSS FULL

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09/885950

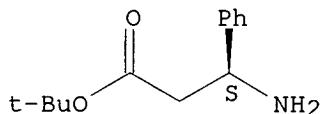
L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN 8-Azabicyclo[3.2.1]octan-3-one, 8-(phenylmethyl)-, oxime (9CI)
MF C14 H18 N2 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Benzenepropanoic acid, .beta.-amino-, 1,1-dimethylethyl ester, (.beta.S)-
(9CI)
MF C13 H19 N O2
CI COM

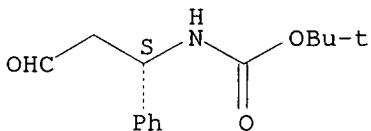
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Carbamic acid, [(1S)-3-oxo-1-phenylpropyl]-, 1,1-dimethylethyl ester (9CI)
MF C14 H19 N O3

Absolute stereochemistry. Rotation (-).

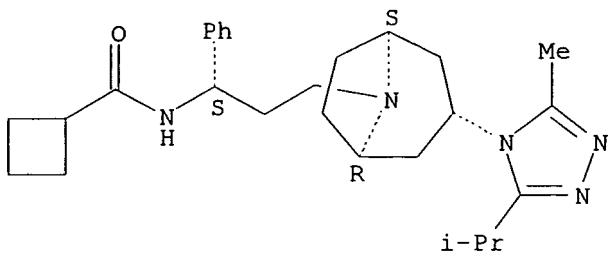


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C27 H39 N5 O

Absolute stereochemistry. Rotation (-).

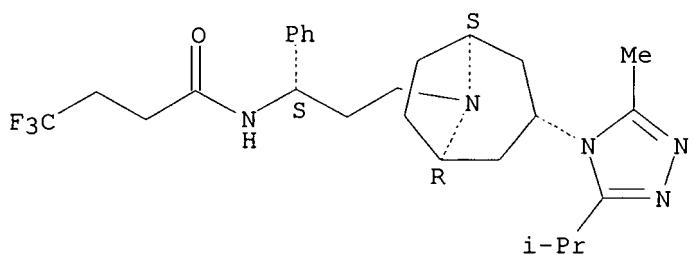
09/885950



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C26 H36 F3 N5 O

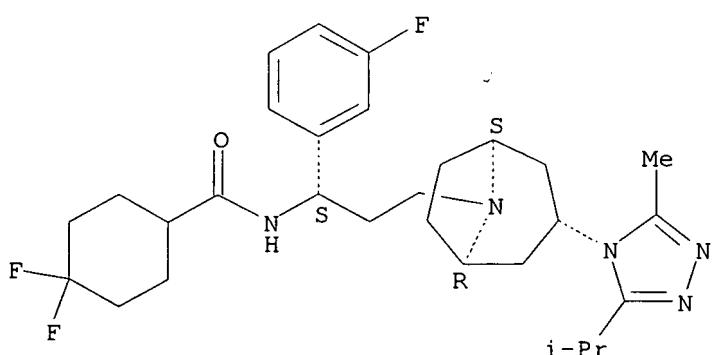
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C29 H40 F3 N5 O

Absolute stereochemistry.

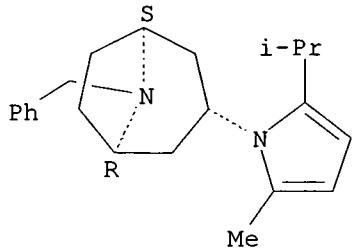


09/885950

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C22 H30 N2

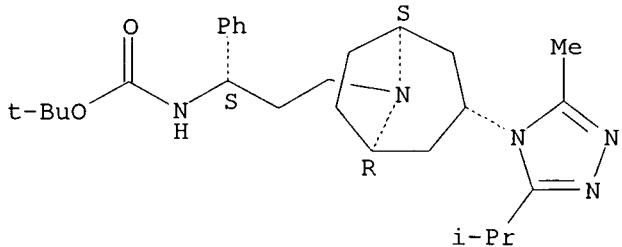
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C27 H41 N5 O2

Absolute stereochemistry.

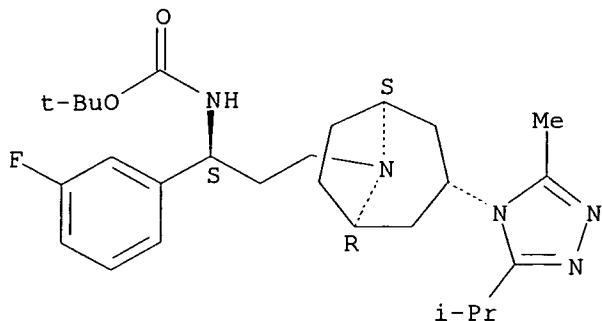


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C27 H40 F N5 O2

Absolute stereochemistry.

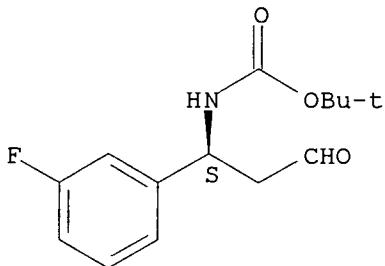
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN INDEX NAME NOT YET ASSIGNED
MF C14 H18 F N O3

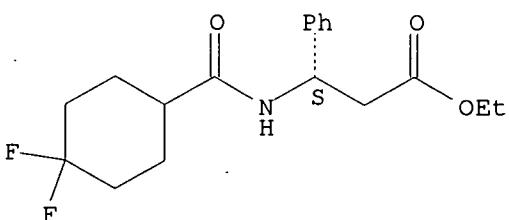
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
* MF C18 H23 F2 N O3

Absolute stereochemistry.

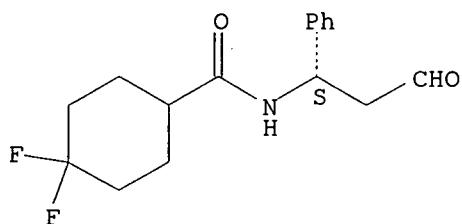


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

09/885950

* L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-oxo-1-phenylpropyl]- (9CI)
MF C16 H19 F2 N O2

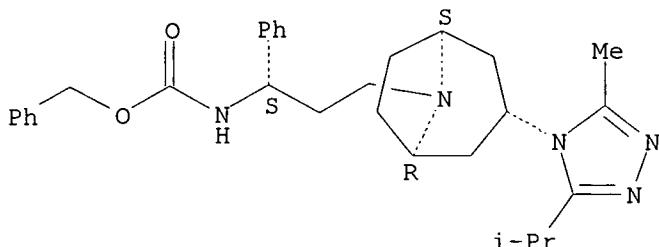
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

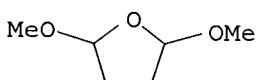
L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C30 H39 N5 O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Furan, tetrahydro-2,5-dimethoxy- (6CI, 7CI, 8CI, 9CI)
MF C6 H12 O3
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS

09/885950

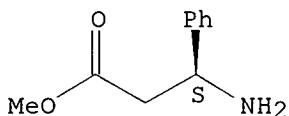
IN Benzenemethanamine, hydrochloride (9CI)
MF C7 H9 N . Cl H
CI COM

H₂N—CH₂—Ph

● HCl

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Benzenepropanoic acid, *.beta.*-amino-, methyl ester, (*.beta.*S)— (9CI)
MF C10 H13 N O2
CI COM

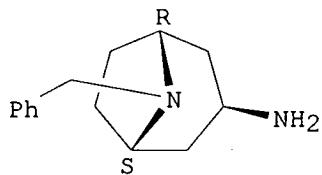
Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(phenylmethyl)-, (3-exo)— (9CI)
MF C14 H20 N2
CI COM

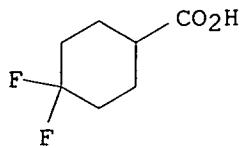
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Cyclohexanecarboxylic acid, 4,4-difluoro- (9CI)
MF C7 H10 F2 O2
CI COM

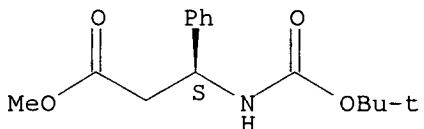
09/885950



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Benzenepropanoic acid, .beta.-[(1,1-dimethylethoxy)carbonyl]amino]-,
methyl ester, (.beta.S)- (9CI)
MF C15 H21 N O4

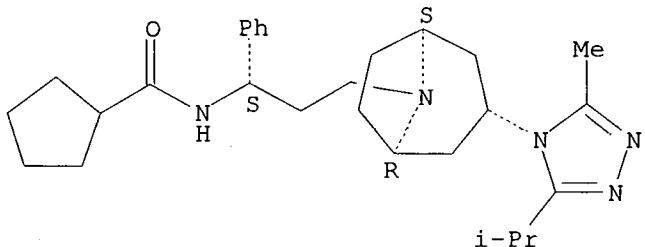
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C28 H41 N5 O

Absolute stereochemistry. Rotation (-).

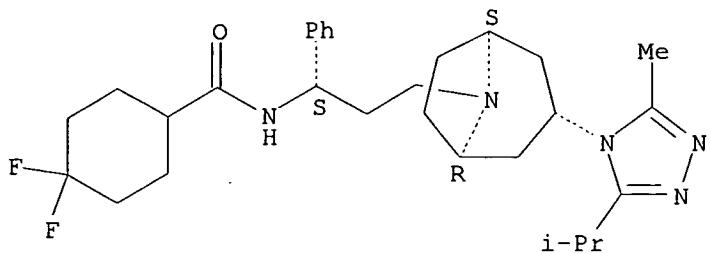


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C29 H41 F2 N5 O

Absolute stereochemistry.

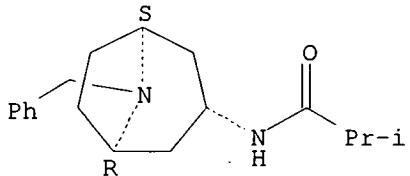
09/885950



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C18 H26 N2 O

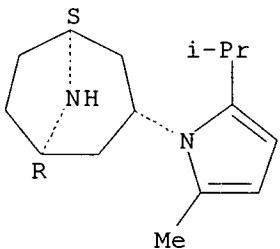
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C15 H24 N2
CI COM

Relative stereochemistry.

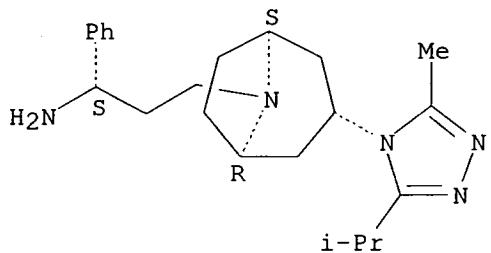


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C22 H33 N5

Absolute stereochemistry.

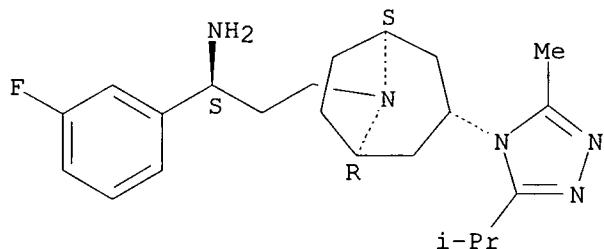
09/885950



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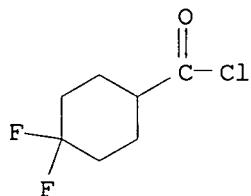
L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C22 H32 F N5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Cyclohexanecarbonyl chloride, 4,4-difluoro- (9CI)
MF C7 H9 Cl F2 O



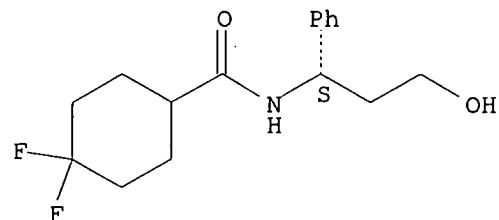
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl]- (9CI)

09/885950

MF C16 H21 F2 N O2

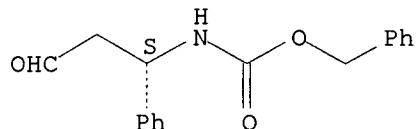
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C17 H17 N O3

Absolute stereochemistry.

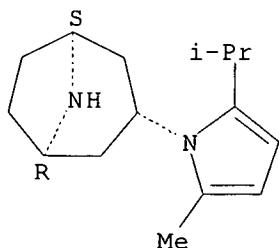


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C15 H24 N2 . C7 H8 O3 S

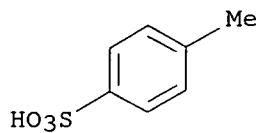
CM 1

Relative stereochemistry.



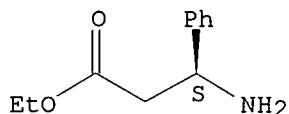
CM 2

09/885950



L2 31 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN Benzenepropanoic acid, β -amino-, ethyl ester, (β -S)- (9CI)
MF C11 H15 N O2
CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

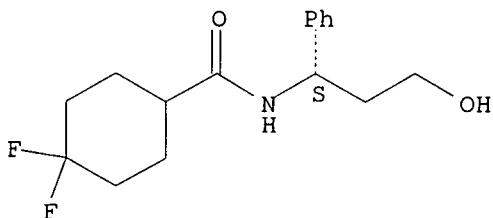
ALL ANSWERS HAVE BEEN SCANNED

=> s 12 and C16H21F2NO2/mf
15 C16H21F2NO2/MF
L3 1 L2 AND C16H21F2NO2/MF

=> d

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN 376348-77-5 REGISTRY
CN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl]-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H21 F2 N O2
SR CA
LC STN Files: CAPLUS

Absolute stereochemistry.



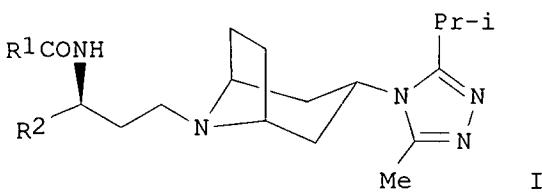
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2001 ACS
 ACCESSION NUMBER: 2001:868452 CAPLUS
 TITLE: Preparation of therapeutic tropane derivatives
 INVENTOR(S): Perros, Manoussos; Price, David Anthony; Stammen,
 Blanda Luzia Christa; Wood, Anthony
 PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
 SOURCE: PCT Int. Appl., 79 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 INT. PATENT CLASSIF.:
 MAIN: C07D451-00
 CLASSIFICATION: 31-3 (Alkaloids)
 Section cross-reference(s): 1, 63
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090106	A2	20011129	WO 2001-IB806	20010509
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			GB 2000-14046	A 20000526
			GB 2000-15835	A 20000627

GRAPHIC IMAGE:



ABSTRACT:

The tropanes I (R1 = C3-6 cycloalkyl optionally substituted by one or more fluorine atoms, C1-6 alkyl optionally substituted by one or more fluorine atoms, C3-6 cycloalkylmethyl optionally ring-substituted by one or more fluorine atoms; R2 = Ph optionally substituted by one or more fluorine atoms) and their pharmaceutically acceptable salts and solvates were prepd. Thus, (1S)-3-[3-(3-isopropyl-5-methyl-4H-1,2,4-triazol-4-yl)-exo-8-azabicyclo[3.2.1]oct-8-yl]-1-phenyl-1-propanamine, prepn. given, was treated with cyclobutanecarboxylic acid in presence of polymer bound N-benzyl-N'-cyclohexylcarbodiimide to give I (R1 = cyclobutyl, R2 = Ph). I had an IC50 value of less than 10nM in the assay for CCR5 binding.

SUPPL. TERM: tropane deriv prepn CCR5 receptor

INDEX TERM: Respiratory tract
(disease; prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: Intestine, disease
(inflammatory; prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: Anti-AIDS agents

Anti-inflammatory agents

Crystal structure

Molecular structure

Respiratory distress syndrome
(prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: Chemokines

ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: Chemokine receptors

ROLE: BSU (Biological study, unclassified); BIOL (Biological study)
(.beta. chemokine receptor CCR5; prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: 376348-65-1P

ROLE: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: 376348-62-8P 376348-63-9P 376348-64-0P 376348-66-2P

ROLE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: 696-59-3, 2,5-Dimethoxytetrahydrofuran 3082-69-7

3287-99-8, Benzylamine hydrochloride 120686-18-2

122665-97-8 376348-71-9 376348-74-2

ROLE: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of tropane derivs. as CCR5 receptor antagonists)

INDEX TERM: 28957-72-4P 37088-66-7P 76272-34-9P 76272-36-1P

135865-78-0P 190189-97-0P 376348-67-3P 376348-68-4P

376348-69-5P 376348-70-8P 376348-72-0P 376348-73-1P

376348-75-3P 376348-76-4P **376348-77-5P**

376348-78-6P 376348-79-7P 376348-80-0P 376348-81-1P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of tropane derivs. as CCR5 receptor antagonists)

EAST - [default.wsp:1]

File View Edit Tools Window Help

Drafts Pending Active L1: (5) perros near manoussos L4: (5) perros near manoussos Failed Saved Favorites Tagged (1) UDC Queue Trash

Search List Browse Queue Clear

DBs USPAT; US-PPGPUB; DERWENT Plurals

Default operator: OR Highlight all hit terms initially

perros near manoussos

BRS f... IS&R... Image Text HTML

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2	<input type="checkbox"/>	<input type="checkbox"/> US 20020032184 A1	20020314	61	Pyrazole derivatives	514/210.2	514/218; 514/235.8;	
3	<input type="checkbox"/>	<input type="checkbox"/> US 20020013337 A1	20020131	26	Tropane derivatives useful in therapy	514/304	546/125	
4	<input type="checkbox"/>	<input type="checkbox"/> US 20010039026 A1	20011108	74	Assay method	435/7.92	435/5	
5	<input type="checkbox"/>	<input checked="" type="checkbox"/> US 6586430 B1	20030701	92	CCR5 modulators	514/235.2	514/256; 514/299;	

Hits Details HTML

Ready